ISSUES IN NONLINEAR, NONSTEADY SOLID COMBUSTION MODELING

B. M. Rasmussen and R. A. Frederick, Jr.
The University of Alabama in Huntsville
Huntsville, AL

ABSTRACT

The focus of the study is a heterogeneous solid combustion model that closely resembles the Beckstead-Derr-Price proposal. Most nonlinear, multiple-flame, separate surface temperature models are valid in the steady-state only, but the current model accounts for nonsteady effects through calculation of two temperature profiles in the solid phase (one for the binder, one for the AP). Some important questions have arisen in the course of model development. The most troubling issue is the over-influence of burning rate on gas-phase heat flux. The problem is reparable by defining the flame heights and temperatures as functions of pressure only, but the authors believe there should be a more phenomenological method for obtaining reasonable results. Another issue is ambiguity in the definition of a "response function" (R_P) for a nonlinear solution. Harmonic inputs do not induce harmonic outputs in nonlinear systems, so the "mean" burning rate term in the standard pressure-coupled frequency response function is not well-defined. The authors explore several ways of calculating frequency response in nonlinear systems, and compare and contrast the answers. Finally, the paper contains some simulations of the response of the propellant to various pressure inputs. Some of the noticed trends are a decreasing R_P amplitude with increasing AP particle diameter, a very slightly increasing R_P amplitude with increasing pressure oscillation magnitude at low frequency, and a decreasing R_P with increasing mean pressure.

INTRODUCTION

BACKGROUND

Most steady-state composite propellant models share a few common characteristics[1]. They typically consider complicated flame interactions that result from the heterogeneous structure of composite propellants (oxidizer particles locked in a binder matrix). Most are one-dimensional, with an averaging scheme that combines the separate mass fluxes into one overall burning rate. Many contemporary models have separate surface temperatures for the binder and oxidizer.

Nonlinear models share some universal characteristics as well. Most incorporate Quasi-Steady gas phase, One-Dimensional (QSOD) assumptions. While a few nonsteady models do consider heterogeneous effects, these models are generally linear and simplified[2]. Conversely, almost all fully nonlinear, nonsteady models assume a homogeneous solid phase (QSHOD), at least in the sense that the solid consists of one substance. A class of newer nonlinear models incorporates variable thermodynamic properties and condensed-phase reactions, but models of this class still only have one surface temperature and temperature profile, together with a single, simplified heat flux from the gas phase[3,4.] The purpose of the current study is to incorporate a fully heterogeneous description of both the flame and solid into a fully nonlinear, nonsteady calculation.

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In addition, the paper contains a discussion of issues and difficulties that have arisen during the course of model development. One issue is that the heterogeneous gas phase produces highly over-damped responses with a full computational treatment, even though it produces reasonable responses when the heat feedback is assumed to be a function of pressure only. Another issue is the definition of a "response function" (R_P) when the response is nonlinear (read: non-harmonic). The paper contains suggestions of how to further explore and overcome these pitfalls in the future. It also presents the results of calculations with various parameters under various conditions.

MODEL DEVELOPMENT

The model is relatively simple and is valid only for mono-modal AP/HTPB propellants, although the techniques used here should extend directly to multi-modal propellants with other oxidizers and inert binders. Mathematically, the model is a system of eight equations, with eight dependent variables:

- Total mass flux
- Oxidizer mass flux
- Binder mass flux
- Height of pre-mixed (AP) flame
- Height of total flame
- Surface temperature of binder
- Surface temperature of oxidizer
- Pre-mixed flame temperature

Figure 1 is a sketch of the propellant surface, illustrating the placement of the variables.

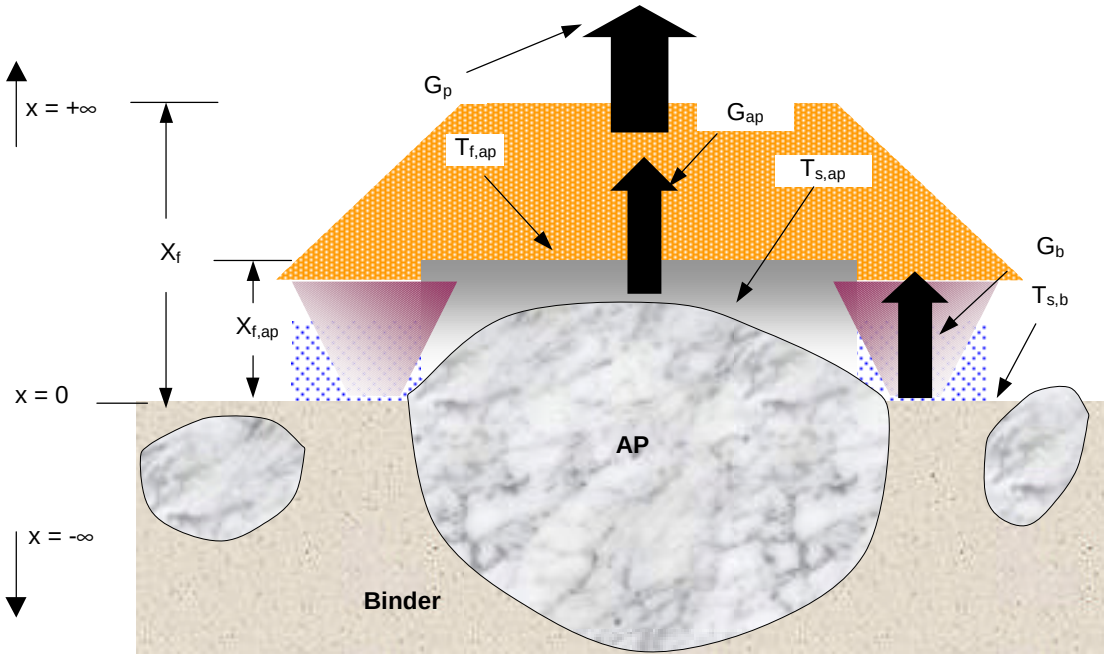

Figure 1: Conceptual Sketch

The equations of the model are below. They have short descriptions in order to conserve space. The mass fluxes of the binder and oxidizer are Arrhenius expressions. The oxidizer expression is

$$G_{ap} = A_{s,ap} \exp\left(-\frac{E_{s,ap}}{RT_{s,ap}} \right) \tag{1}$$

and the binder expression is

$$G_{b} = A_{s,b} \exp\left(-\frac{E_{s,b}}{RT_{s,b}} \right) \tag{2}$$

The total combined mass flux of the propellant is an algebraic combination of the mass fluxes of the binder and oxidizer. It is based on a time-averaged approximation of linear burning. The result is

$$G_{p} = \frac{1}{\frac{\alpha_{ap}}{G_{ap}} + \frac{1-\alpha_{ap}}{G_{b}}} \tag{3}$$

The pre-mixed AP flame is a second-order kinetics-dominated flame, so it is related to the inverse square of the pressure. It is also a linear function of oxidizer mass flux. The pre-mixed flame height is

$$x_{f,ap} = \frac{G_{ap}}{P^{2} A_{g,ap} \exp\left(-\frac{E_{g,ap}}{RT_{f,ap}} \right)} \tag{4}$$

The expression for total flame height is somewhat more complicated. It, too, has a reaction component that is related to the inverse square of the pressure, but it also has a diffusion component with both turbulent and laminar coefficients. The reaction component (corresponding to a reaction flame above the binder) is actually a separate entity, but the sum of the reaction and diffusion components is really all that is necessary for calculation. Thus, the sum has the label "x_f". For a more complete derivation of the following equation, see Rasmussen et al[5]. The total flame height is

$$x_{f} = \frac{\dot{m}_{p} D_{ap}^{*\,2}}{A_{diff}\left[D_{0} T_{f,ap}^{\beta-1} \frac{M}{R} + K\dot{m}_{p} D_{ap}^{*} \left(\tan^{-1}\left(C_{1}C_{2}\right) + \tan^{-1}\left[C_{2}\left(\frac{1}{x_{r}} - C_{1} \right) \right] \right) \right]} + \frac{\dot{m}_{p}}{P^{2} A_{r} \exp\left(-\frac{E_{r}}{RT_{f}} \right)} \tag{5}$$

where D^*_{ap} is a characteristic AP particle diameter, related to the AP mass flux, initial AP diameter, and total propellant mass flux:

$$D_{ap}^{*} = \frac{2D_{ap}}{\sqrt{6\frac{\rho_{p} G_{ap}}{\rho_{ap} G_{p}}}} \tag{6}$$

Energy balances from far below the surface (x = -8) to just above the surface (x = 0^+) provide equations for the surface temperatures: The energy balance in the AP is the following (based on pure conduction into the surface):

$$G_{ap}C_{p,s,ap}T_i + \lambda_{g,ap}\left.\frac{\partial T}{\partial x}\right|_{x=0^+} + G_{ap}q_{v,ap} = G_{ap}C_{p,g,ap}T_{s,ap} + \int_{-\infty}^{0}\rho_{s,ap}C_{p,s,ap}\frac{\partial T}{\partial t}\partial x \tag{7}$$

Assume an exponential temperature profile above the surface in order to calculate the ∂T/∂x terms. the exponential profile above the AP is

$$T(x) = \left(T_{s,ap} - T_{f,ap}\right)\exp\left(-\nu\frac{x}{x_{f,ap}}\right) + T_{f,ap} \tag{8}$$

Solving for $T_{s,AP}$ yields

$$T_{s,ap} = \frac{G_{ap}C_{p,s,ap}T_i + \lambda_{g,ap}T_{f,ap}\dfrac{\nu}{x_{f,ap}} + G_{ap}q_{v,ap} - \displaystyle\int_{-\infty}^{0}\rho_{s,ap}C_{p,s,ap}\frac{\partial T_{ap}(t,x)}{\partial t}dx}{G_{ap}C_{p,g,ap} + \lambda_{g,ap}\dfrac{\nu}{x_{f,ap}}} \tag{9}$$

Proceeding with an almost identical method, the expression for the surface temperature of the binder is

$$T_{s,b} = \frac{G_bC_{p,s,b}T_i + \lambda_{g,b}T_f\dfrac{\nu}{x_f} + G_bq_{v,b} - \displaystyle\int_{-\infty}^{0}\rho_{s,b}C_{p,s,b}\frac{\partial T_b(t,x)}{\partial t}dx}{G_bC_{p,g,b} + \lambda_{g,ap}\dfrac{\nu}{x_f}} \tag{10}$$

Another energy balance, from x_{ap} to x_f, defines the temperature of the pre-mixed flame. This energy balance does not include the integral (nonsteady) term, because the gas phase is quasi-steady by assumption:. The final result is the following:

$$T_{f,ap} = \frac{T_f\left[G_pC_{p,g,p} + \dfrac{\nu\lambda_{g,p}}{x_f - x_{f,ap}}\right] - G_pq_f}{G_pC_{p,g,p} + \dfrac{\nu\lambda_{g,p}}{x_f - x_{f,ap}}} \tag{11}$$

To reiterate, the model is a system of eight equations to be solved simultaneously (Equations (1), (2), (3), (4), (5), (9), (10), and (11)). At steady-state, the integral terms are zero, and it is possible to solve the equations without too much difficulty using commercial mathematical software.

TRANSIENT SOLUTION METHOD

In order to extend the model to nonsteady situations, one must calculate the integral terms in Equations (9) and (10). This requires a computation of the temperature profile in the binder and AP. The $\partial T/\partial t$ terms derive from the transient heat conduction equation with constant thermal properties, i.e.,

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} - r \frac{\partial T}{\partial x} \tag{12}$$

One can use a method similar to the Crank-Nicolson approach, which averages finite-difference derivatives at known time t_i and unknown time t_{i+1}. With boundary conditions $T|_{x=0} = T_s$ and $T|_{x=-\infty} = T_i$, the new temperature profile is the solution to a tri-diagonal matrix equation. The new temperature profile at time t_{i+1} is a function of the temperature profile at time t_i and a new (to be iterated upon) surface temperature. That is,

$$\begin{aligned} \int_{-\infty}^{0} \rho_{s,b} C_{p,s,b} \frac{\partial T_b}{\partial t} dx &\equiv f\left(T_{s,b,new}, \text{"previous binder temperature profile"}\right) \\ \int_{-\infty}^{0} \rho_{s,ap} C_{p,s,ap} \frac{\partial T_{ap}}{\partial t} dx &\equiv f\left(T_{s,ap,new}, \text{"previous AP temperature profile"}\right) \end{aligned} \tag{13}$$

The starting point for the nonsteady model is a steady-state solution of Equation (12). is a plot of the steady-state temperature profiles in the binder and oxidizer for a (90,80/20,298)* propellant. Near the surface, the x-spacing decreases exponentially to account for faster changes in the temperature profile.

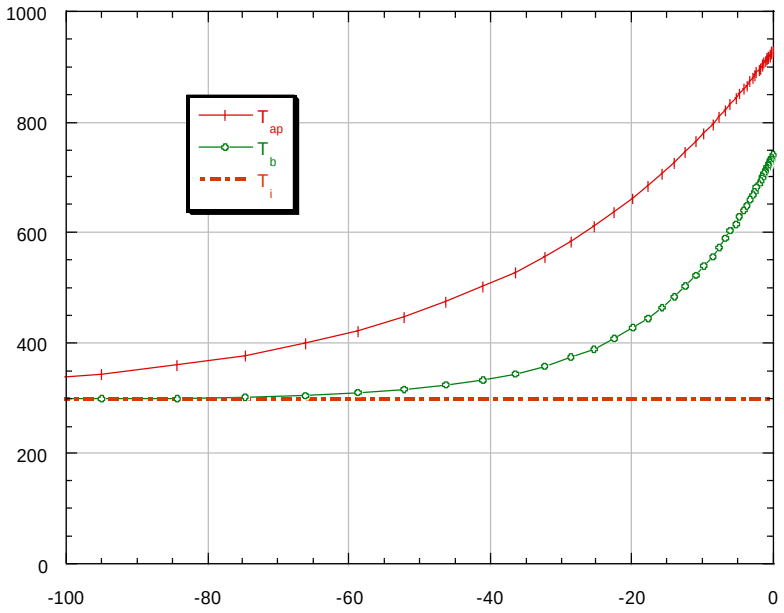

Figure 2: Steady-State Temperature Profiles

* (a,b/c,d) implies that the propellant has "a" µm AP particle diameter, "b" % AP by mass, "c" % binder by mass, and "d" initial temperature.

As in the steady-state version, the model is eight equations to be solved simultaneously, but two of the equations now require the solution of a tri-diagonal matrix equation representing temperature profile changes. The model is solved using Mathcad 7.0.3 commercial mathematical software, with some of the more computationally demanding routines written in Microsoft Visual C++.

RESULTS AND DISCUSSION

STEADY-STATE RESULTS

Figure 3 is a plot of burning rate vs. pressure. It shows the steady-state model predictions as compared to experimental data for two propellants- (5,80/20,298) and (90,80/20,298). It also shows a theoretical prediction for (50,80/20,298) and (200,80/20,298) propellant. Experimental data come from ultrasonic tests at ONERA[6]. Figure 4 is a plot of flame height and pre-mixed flame temperature as a function of pressure for a (90,80/20,298) propellant. These curves define the heat flux out of the gas phase.

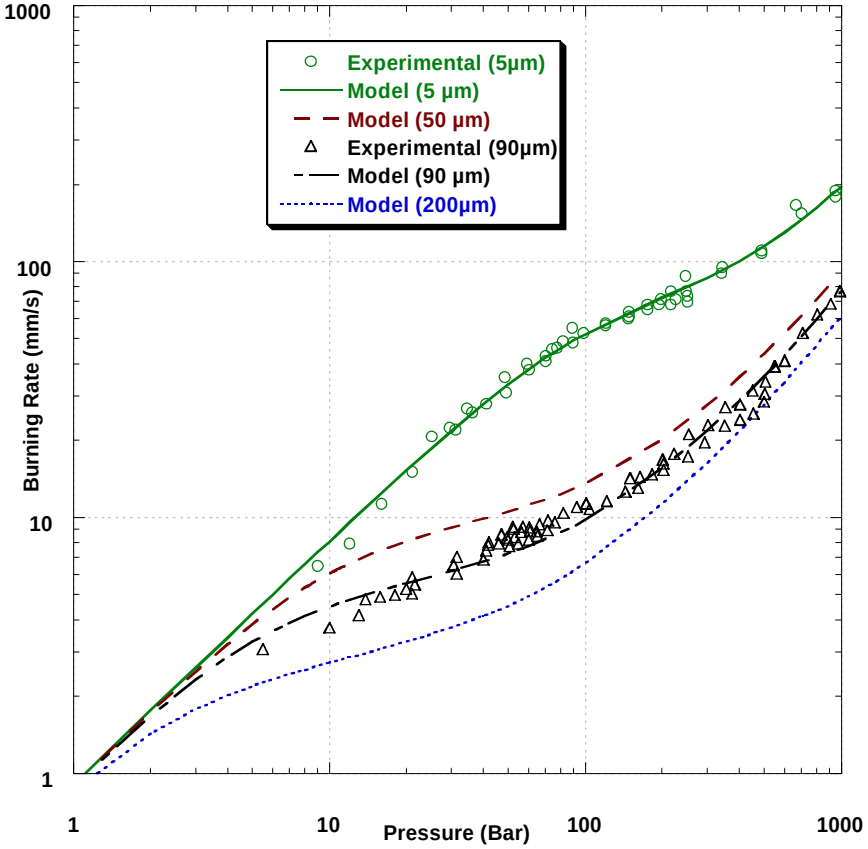

Figure 3: Burning Rate vs. Pressure for Three Formulations

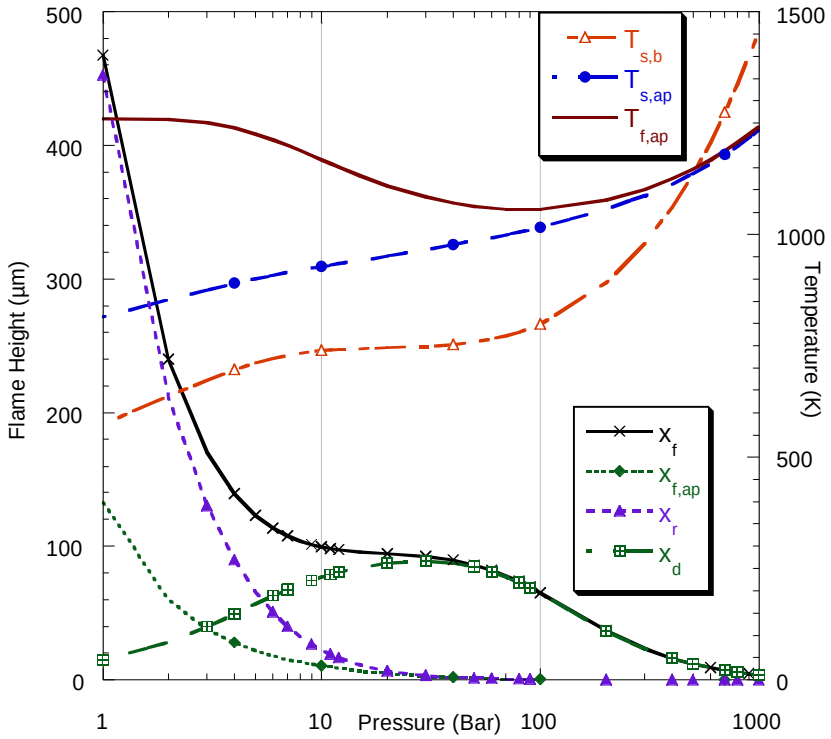

Figure 4: Flame Parameters as a Function of Pressure

NONSTEADY ISSUES

Unfortunately, the current gas phase model seems to imply an over-dependence of heat feedback on burning rate. The burning propellant system has one source of capacitance (the thermal lag in the solid phase) and it has two sources of damping (heat of vaporization at the surface, and "dragging" of the gas phase due to its dependence on burning rate). In other words, both the heat flux *out of* the gas phase and the heat flux *into* the solid phase are functions of burning rate.

Some analyses anticipate that the heat flux out of the gas phase is purely a function of pressure[7], but this assumption appears to be unrealistic, especially in light of the effect of burning rate dependence on the current model. Other analyses *do* include the effect of burning rate on flame heat feedback, but they incorporate simplified, homogeneous flame models with single surface temperatures[8].

Despite problems with burning rate dependence, it is still possible to obtain reasonable results from the current model by making a curve-fit of $x_{f,ap}$, $T_{f,ap}$, and x_f from the steady-state model with respect to pressure (as in Figure 4), then using the curve fits in the nonsteady version. This method forces the heat-feedback out of the gas phase to be solely a function of pressure, effectively eliminating one of the damping paths in the system. As mentioned, this is a questionable approximation, but it does allow for reasonable results, which in turn allow for an exploration of heterogeneous effects on the response.

Figure 5 is a plot of the response of the burning rate to a step input using several different calculation methods on a (90,80/20,298) propellant. "Full Calculation" means that the variable in question comes from instantaneous calculation of either one of Equations (4), (5), or (11), with or without an explicit reaction height calculation. "Curve Fit" means that the variable in question comes from a curve fit to the steady-state data, and thus is a function of pressure only. Figure 6 shows the effect of various calculation methods on the frequency response. All curves in Figure 6 come from the peak-average method, as discussed later.

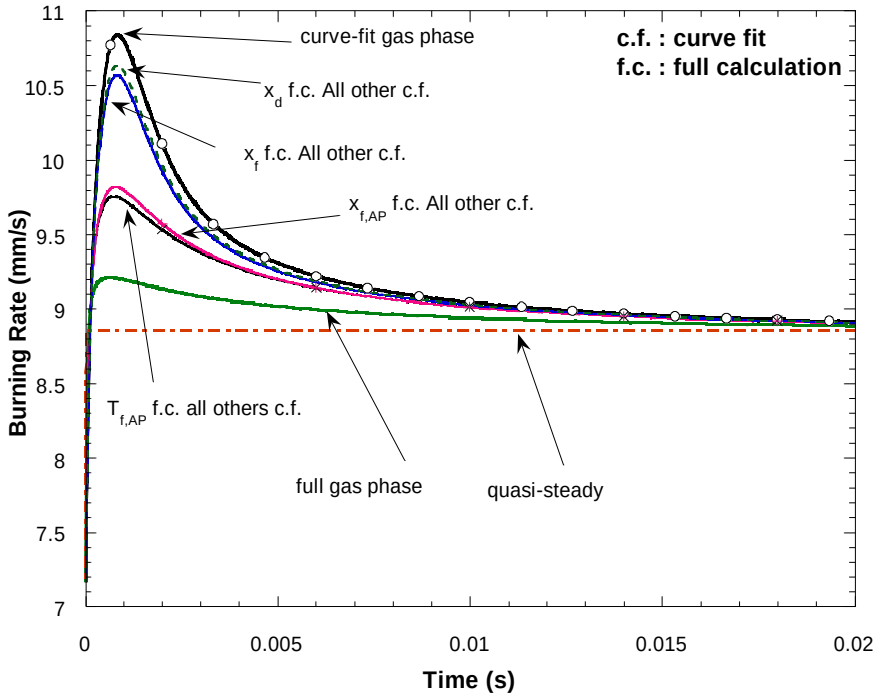

Figure 5: Response to a Step Input with Various Calculation Methods

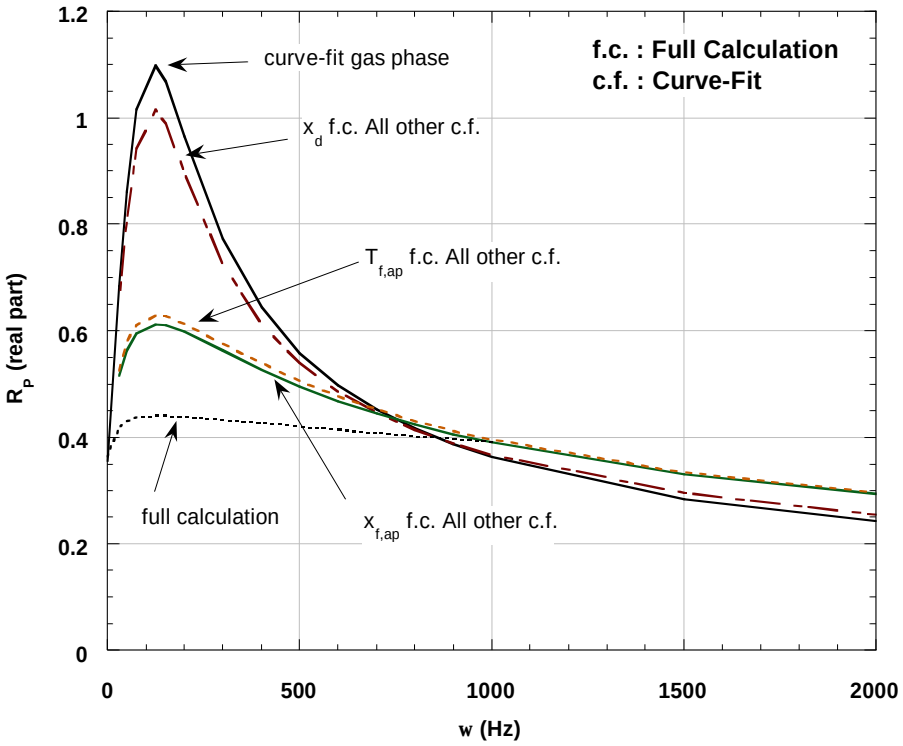

Figure 6: Frequency Response with Various Calculation Methods

From observation of Figure 5 and Figure 6, the variables $T_{f,ap}$ and $x_{f,ap}$ seem to cause the largest deficit in transient response. The equations that describe these two variables, however, are neither new nor particularly uncommon in heterogeneous steady-state models. The authors believe that there should be a phenomenological explanation for the over-dependence and recommend it as an area for future study.

Clearly, the curve-fitting of the gas phase greatly enhances the response magnitude and allows for further study. While it may not be a perfect simplification, pressure-dependent-only gas phase heat-feedback is an assumption in all simulations for the rest of the paper.

Given a model that produces reasonable results, one obvious question arises: How does one calculate a 'response function' with a completely nonlinear model? Linear systems, of course, have harmonic outputs in response to harmonic inputs. Moreover, the oscillatory mean of the harmonic output is the steady-state solution. Nonlinear models are not as clean.

To illustrate the point, consider two simulations. Each simulation for the remainder of the paper runs to either 10 "time constants", or 10 pressure oscillations, whichever is greater. The "time constant" is the maximum characteristic response time of the system (either AP or binder):

$$\tau = \frac{\alpha}{r^2} \tag{14}$$

Figure 7 is a plot of the final oscillation of a (90,80/20,298) propellant, given a 2 bar pressure oscillation around a mean of 10 bars at 500 Hz. Note the slight difference between the steady-state value, the mean value, and the peak-average value, even after 10 time constants. Also, notice that the oscillation in Figure 7 is not quite harmonic.

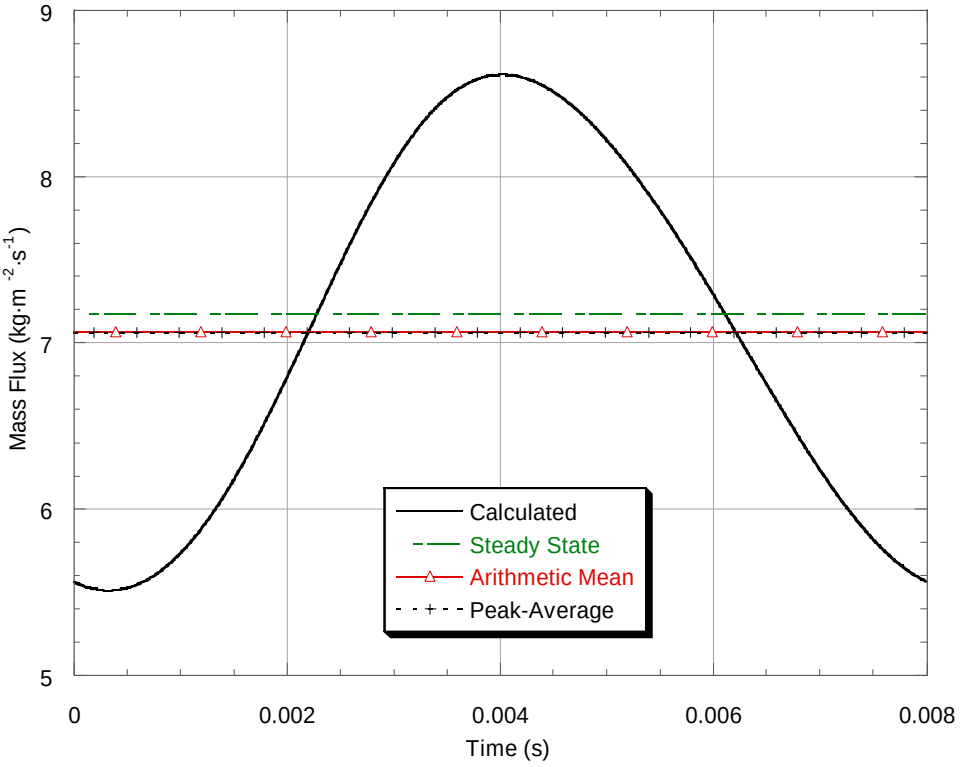

Figure 7: Final Oscillation of Burning Rate, Given Sinusoidal Pressure Input

Figure 7 illustrates a serious problem in calculating R_P. The definition of R_P is

$$R_p = \frac{r'/\bar{r}}{P'/\bar{P}} \tag{15}$$

What are r´ and $\bar{r}$ in the above expression? For linear models, there is no difficulty— the mean and steady-state are identical, and the r´ can be either the maximum burning rate or the minimum burning rate, since the output is sinusoidal. In a nonlinear model, however, the output is not sinusoidal, nor does it have a "mean" at the steady-state value. Given the non-harmonic function shown in Figure 7, there are at least five methods for calculating the R_P:

1) $\bar{r}$ = arithmetic mean; r´ = max.
2) $\bar{r}$ = arithmetic mean; r´ = min.
3) $\bar{r}$ = (r_{min} + r_{max})/2; r´ = max. or min.
4) $\bar{r}$ = steady-state at $\bar{P}$; r´ = max..
5) $\bar{r}$ = steady-state at $\bar{P}$; r´ = max.

Method 3 seems to be the preferred method, because it gives an R_P that is typically between the extremes of the other two, and because it returns only one value of R_P using the same "mean". Figure 8 is a plot of R_P vs. frequency using all of the calculation methods on a (90,80/20,298) propellant. The bottom two lines show the percentage difference between the steady-state $\bar{r}$ and the $\bar{r}$'s used in methods 1, 2, and 3. In all the following plots, the point at "zero frequency" is simply a calculation without any of the nonsteady terms. (The model, as written, cannot accept an input of 0 for the frequency, because it causes singularities in the code.)

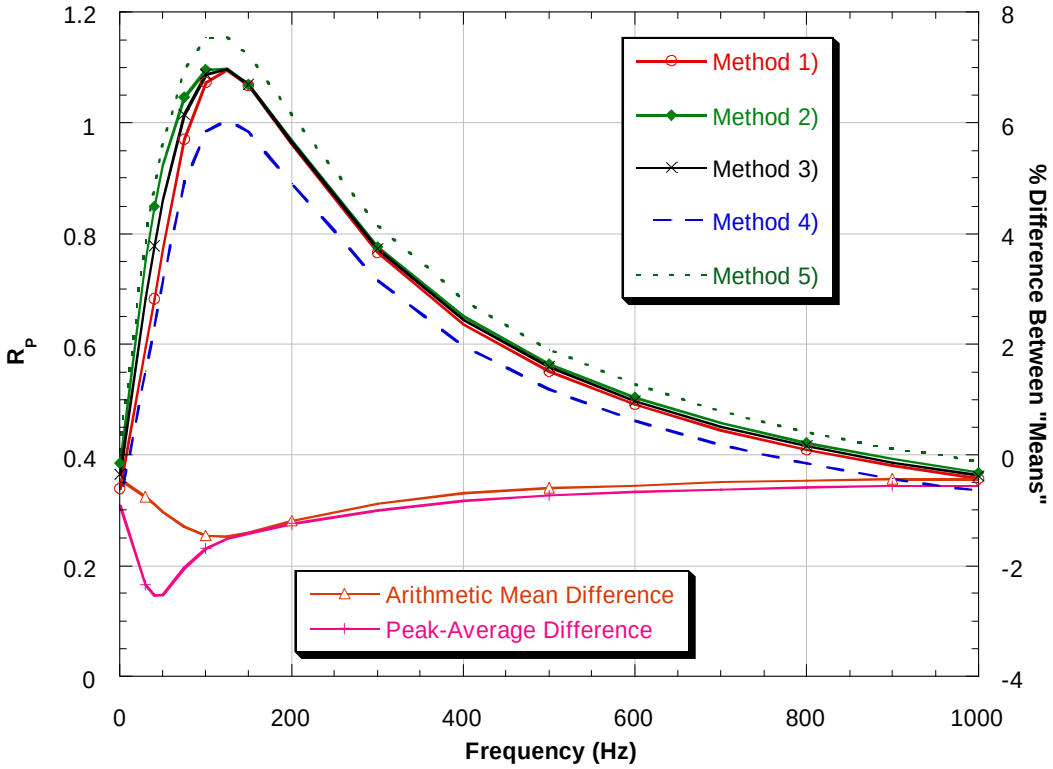

Figure 8: Various Methods of Calculating R_P

NONSTEADY RESULTS

Figure 9 shows R_P vs. frequency for various AP particle diameters at 20% oscillation amplitude, Figure 10 shows R_P vs. frequency for various mean pressures with a (50,80/20,298) propellant and 20% oscillation amplitude, and Figure 11 shows R_P vs. frequency for various oscillation magnitudes at 10 bar mean pressure. All calculations are from method 3.

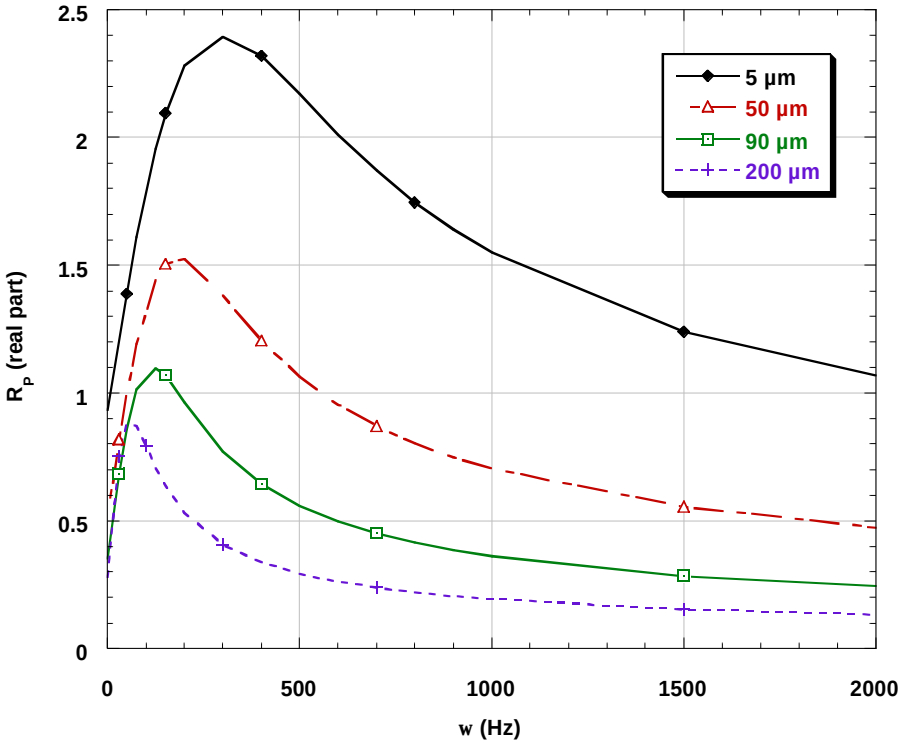

Figure 9: Effect of AP Particle Diameter on R_P

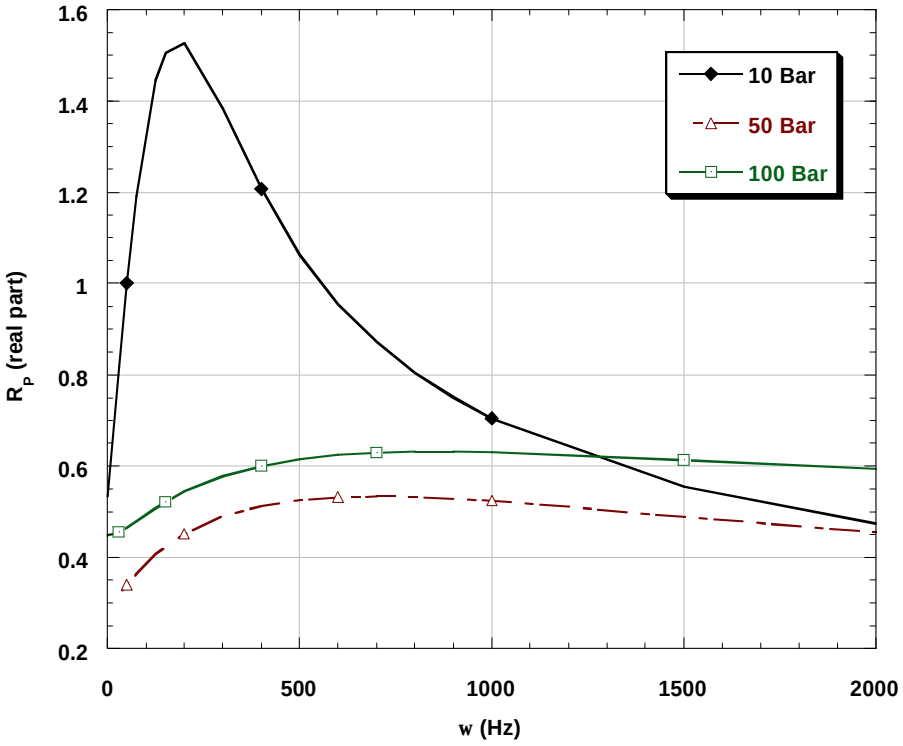

Figure 10: Effect of Mean Pressure on R_P

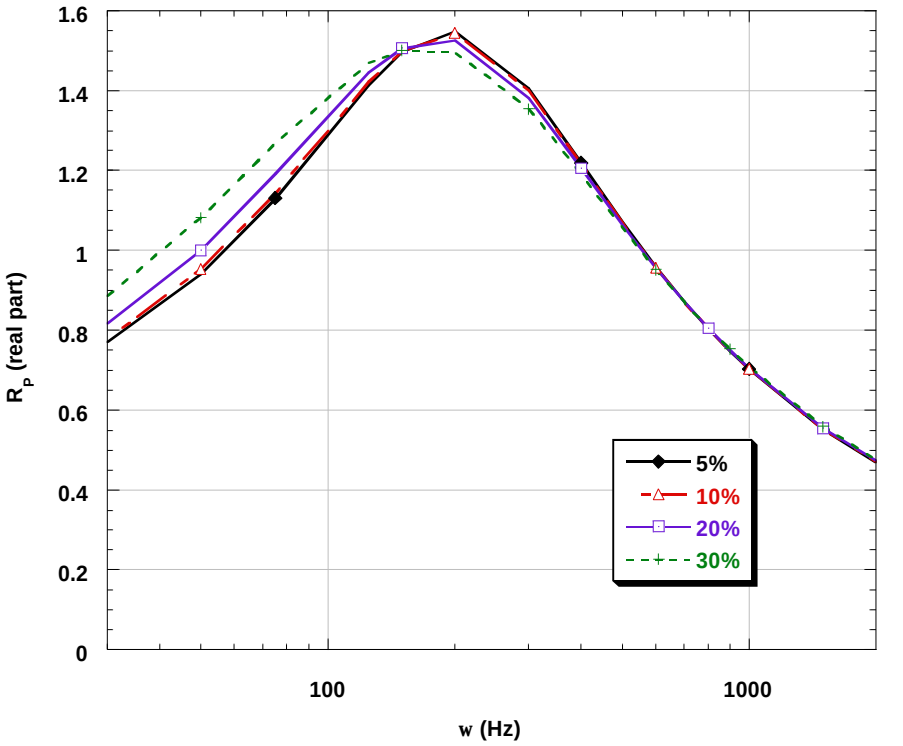

Figure 11: Effect of Oscillation Magnitude on R_P

CONCLUSIONS

Two distinct issues have become apparent during the development of the model described in this paper. The most important issue is the apparent over-influence of burning rates on the gas-phase heat feedback. To the authors' knowledge, no one has yet attempted to apply a separate-surface temperature multiple flame model in a nonlinear, nonsteady simulation, and the over-dependence in the current model is troubling. Given the results of the study, one can make several possible conclusions:

- The model is fundamentally correct, and a "tweaking" will eliminate the over-dependence.
- Multiple flame models such as these are incapable of simulating nonlinear, nonsteady combustion.
- Other factors besides the thermal profile relaxation effect are significant in combustion instability, and all models that rely solely on the thermal profile relaxation will under-estimate the response.

The authors recommend further study in this area. In the meantime, it is possible to obtain results by fitting the gas phase and tying it to the pressure only.

The next obvious issue is the problematic definition of R_P in nonlinear situations. Out of the several techniques reviewed, the recommended method is a "peak-average" definition of mean burning rate. This method, coupled with gas-phase curve-fitting, gives the results shown in the "Nonsteady Results" section.

A few trends become apparent in the plots of nonsteady results. First, amplitude of frequency response definitely becomes larger with decreasing AP particle diameter. This effect may be due to the lessening influence of diffusion flames. With very small particle diameter, the propellant flame structure is nearly homogeneous.

Second, higher mean pressures tend to lower the response amplitude and shift it to higher frequencies. The temperature profiles are much shorter at high pressure, and the burning rates are much higher. Thus, the characteristic response times of the AP and binder are much shorter. This hypothesis does not agree, however, with the fact that response is inversely proportional to AP particle diameter, because propellants with small AP particle diameters typically burn faster than propellant with large AP crystals. Further study is necessary here.

Third, oscillation magnitude does not seem to have a significant effect on the propellant response, at least not for magnitudes under 30% using the peak-average technique of response calculation. One would expect oscillation magnitude to induce a larger difference with methods 1, 2, 4, and 5.

NOMENCLATURE

A : pre-exponential factor
A_{diff} : diffusion constant
C : constant
C_P : constant-pressure specific heat
D : diffusion coefficient
D : AP particle diameter
E : activation energy
G : mass flux
K : Turbulent diffusion constant
M : molecular weight
P : pressure
q : specific energy release (+ exothermic)
R : universal gas constant
r : linear burning rate
T : temperature
t : time
x : distance

α : oxidizer mass fraction, or thermal diffusivity
β : exponential diffusion constant
λ : thermal conductivity
ν : exponential growth factor
ρ : density
σ_p : initial temperature sensitivity

τ : characteristic response time

$( )_{ap}$: ammonium perchlorate
$( )_b$: binder
$( )_c$: condensed phase
$( )_f$: flame
$( )_g$: gas-phase
$( )_i$: initial conditions
$( )_p$: propellant
$( )_P$: pressure
$( )_s$: surface, or solid
$( )_v$: vaporization
$\overline{( )}$: steady-state, or mean
$( )'$: differential
$( )_0$: initial

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